Self-avoiding walks including next-nearest-neighbor steps

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A self-avoiding-walk series on lattices of high effective coordination number in two dimensions are obtained by allowing next-nearest-neighbor steps in addition to nearest-neighbor steps. The dependence of the connective constant of self-avoiding walks on the lattice coordination number is studied by means of standard methods of series analysis.

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Self-avoiding walks (SAWs) have attracted much theoretical attention in recent years owing to their numerous applications in physical and biological sciences. For example, configurational properties of a dilute macromolecule in a good solvent can be modeled by SAWs [1, 2]. It is generally believed that the asymptotic behavior of C_N, the number of allowed N-step walks on a given lattice and starting from a given site, is

$$C_N \sim \mu^N N^{\gamma-1}(1 + BN^{-\Delta} + CN^{-1} + \cdots), \quad (1)$$

where the connective constant μ depends on both the coordination number and the lattice chosen, while the exponent γ is believed to be universal and, for two-dimensional systems, equal to 43/32 [3]. Although there has been extensive work done to determine Δ, the correction-to-scaling exponent, its value remains controversial [4–8].

In this Brief Report, we address the following question: How does an increase in coordination number z affect the connective constant μ? This question is of fundamental interest in trying to understand the relationship between geometrical structure and critical phenomena. In addition, there is considerable interest in polymers containing vertices of high functionality (degree) including stars with many legs [9]. In order to study lattice models of such polymers, lattices with high effective coordination number are required. Barrett and Pound [10] have used a different method of generating high effective coordination number lattices and our work is complementary to theirs. From the critical phenomena point of view, work on polymer topologies containing vertices of high degree will provide critical tests of the understanding developed through scaling theory [11] and the application of conformal covariance theory [12]. Tests in two dimensions, where conformal covariance theory provides exact results for critical exponents, are particularly critical. Due to the inherent difficulties in dealing with uniform structures with a large number of branch points [13], an accurate estimate of μ is highly desirable when making such tests. Rigorous results show that μ is independent of the polymer topology chosen [14]. Consequently, accurate estimates of μ obtained from SAWs on high effective coordination number lattices are likely to be of considerable utility when studying more complex structures on these lattices.

To answer the question posed above, we study the changes in μ caused by the inclusion of next-nearest-neighbor (NNN) steps on the square (sq) and triangular (tr) lattices. For the square lattice this amounts to increasing z from 4 to 8 and for the triangular lattice the increase is from 6 to 12. The values of μ for the triangular, the square, and the honeycomb (hc) lattices using nearest-neighbor (NN) steps only used below were taken from published sources [15, 16, 3]. For the square lattice we have enumerated walks with up to 15 vertices and for the triangular lattice we have enumerated walks with up to 13 vertices. Copies of the series coefficients generated in this way are available from the authors on request. Our methods of series analysis are standard and consist of Neville table analysis, D log Padé approximants, and the Baker-Hunter confluent singularity analysis [17]. Estimates of the critical exponent obtained by these methods were consistent with the expected value of $\gamma = 43/32$. Central estimates of μ were then biased to this value of γ. Overall estimates of the connective constants obtained from these methods are

$$\mu(\text{trNNN}) = 9.400 \pm 0.005,$$
$$\mu(\text{sqNNN}) = 5.836 \pm 0.001.$$

These estimates are based primarily on the D-log Padé and Baker-Hunter analyses as the Neville tables tend to give consistent but less precise results. The values of μ may be compared with the corresponding values for lattices on which only nearest-neighbor steps are allowed:

$$\mu(\text{tr}) = 4.1508 \pm 0.0001,$$
$$\mu(\text{sq}) = 2.638\ 16 \pm 0.000\ 01,$$
$$\mu(\text{hc}) = \sqrt{2+\sqrt{2}} \qquad \text{(exact)}.$$

In addition we have analyzed the auxiliary series generated by taking the ratios of coefficients in the series of interest and the corresponding coefficient in the series for the same lattice but with nearest-neighbor steps only. The usefulness of such a *ratio of coefficients* analysis is easy to demonstrate: Let C_N and C_N^R be the Nth coefficients of the aforementioned series. Then the generating function of the series of ratios of coefficients

$$G(x) = \sum_{N=0} \frac{C_N}{C_N^R} x^N \quad (2)$$

has the exponent $\gamma = 1$. Consequently, standard Padé approximants as well as the methods used in the case of the original series yield an accurate estimate of the corresponding ratio of connective constants:

$$\frac{\mu(\text{trNNN})}{\mu(\text{tr})} = 2.268 \pm 0.005,$$
$$\frac{\mu(\text{sqNNN})}{\mu(\text{sq})} = 2.212 \pm 0.005,$$
$$\frac{\mu(\text{tr})}{\mu(\text{hc})} = 2.2464 \pm 0.0001.$$

The last entry is based on the values of $\mu(\text{tr})$ and $\mu(\text{hc})$ (with only NN steps) given earlier in this paper.

Note that the ratios are almost constant and about 10% higher than the random-walk value. In contrast, the corresponding values of these ratios when a Bethe approximation is used (i.e., a random walk with no immediate back steps) vary from 2.2 to 2.5 for these lattices. For completeness, we note the following ratios for three-dimensional lattices where sc denotes simple cubic and tet denotes tetrahedral:

$$\frac{\mu(\text{bcc})}{\mu(\text{tet})} = 2.27,$$
$$\frac{\mu(\text{fcc})}{\mu(\text{sc})} = 2.14,$$
$$\frac{\mu(113)}{\mu(\text{fcc})} = 2.24,$$
$$\frac{\mu(112)}{\mu(\text{fcc})} = 2.23.$$

These values are based on published values of μ for the individual lattices [16, 10, 5]. The error estimates are negligible at the number of figures quoted here.

With the exception of the slightly lower value obtained for the fcc-sc pair, these ratios show a remarkable lack of dependence on coordination number or dimensionality. The slight variations seen presumably depend on the fine details of the lattice structure. The variation with coordination number is certainly significantly less than indicated by the Bethe approximation.

From Eq. (1) the mth moment of the generating function for SAWs is expected to have the form

$$f(x) = \sum_{N=0} C_N x^N N^m = (1-\mu x)^{-\gamma_e}[A + B(1-\mu x)^{\Delta} + C(1-\mu x) + \cdots]. \quad (3)$$

In the above equation, the effective exponent is given by $\gamma_e = \gamma + m$. Numerical evidence is consistent with the exact value of γ predicted by conformal covariance theory. However, there has been considerable controversy over the value of the correction to scaling exponent Δ [4–8].

Here we report results from Baker-Hunter analyses of self-avoiding-walk series on the square and triangular lattices when next-nearest steps are allowed. For completeness, we have also analyzed the corresponding series when only nearest-neighbor steps are allowed. The Baker-Hunter method involves the construction of an auxiliary function [18, 17]

$$\chi(y) = \sum_n g_n y^n = \frac{A}{1-y\gamma_e} + \frac{B}{1-(\gamma_e-\Delta)y} + \frac{C}{1-(\gamma_e-1)y} + \cdots. \quad (4)$$

In addition to enabling the determination of the exponents, the Baker-Hunter method also provides estimates of the amplitudes A, B, and C, if the input series is long enough. If the second moment of the generating function is analyzed, all of the series, except that for the triangular lattice with next-nearest-neighbor steps, exhibit a pole corresponding to $1.00 \leq \Delta \leq 1.04$. A separate analytic term is not resolved by the approximants. In the first moment series for the triangular lattice with nearest-neighbor steps only and the square lattice with next-nearest-neighbor steps a substantially higher value of $1.2 \leq \Delta \leq 1.4$ is obtained. This is also true of the first moment series for the square lattice with only nearest-neighbor steps if only the first 20 terms of the series are used. However, approximants based on all 30 of the currently available series give a value of $\Delta \approx 1.08$. Again a separate analytic term is not resolved by the approximants. In view of this, the higher values given by the other first moment series should be regarded as short series effects.

The estimates of Δ obtained in this way may indicate that the true value is slightly above 1.0. The values obtained are then effective values representing the presence of both the analytic and nonanalytic correction terms in the original series. In an attempt to separate the analytic and nonanalytic correction exponents, we have considered an alternative method for the determination of Δ. This involves the subtraction of the leading pole term of χ thereby obtaining a function

$$\Psi(y) = \chi(y) - \frac{A}{1-y\gamma_e}. \quad (5)$$

This function is easy to construct once $\mu = 1/x_c$ and the amplitude A are accurately known. In our case, values from the previous analysis must be used. The Ψ function constructed in this way exhibited only a single pole on the real axis (within a reasonable range of values) for each series considered and gave estimates of Δ consistent with those obtained from the ordinary Baker-Hunter analysis.

The confluent singularity analyses for the triangular lattice with next-nearest-neighbor steps was performed as described above. However, the estimates of Δ were all in a lower range than that found above ($0.6 \leq \Delta \leq 1.0$). The convergence of the approximants for this series appeared to be poorer than that for the other series and probably even this rather broad estimate should not be treated as reliable until further terms in the series have been enumerated and analyzed.

Overall our results appear to favor a Δ very close to

but larger than 1. A very recent Monte Carlo study, using large chains, obtains effective values of Δ slightly below 1. However, the error bars are large enough to allow a value slightly larger than 1 [8]. A more precise estimate of Δ does not appear to be possible with the series currently available.

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[1] P.-G. de Gennes, *Scaling Concepts in Polymer Physics*, 3rd ed. (Cornell University, Ithaca, 1988).
[2] K.F. Freed, *Renormalization Group Theory of Macromolecules* (Wiley, New York, 1987).
[3] B. Nienhuis, J. Stat. Phys. **34**, 731 (1984).
[4] J.C. Le Guillou and J. Zinn-Justin, Phys. Rev. Lett. **39**, 95 (1977); Phys. Rev. B **21**, 3976 (1980).
[5] T. Ishinabe, Phys. Rev. B **39**, 9486 (1989).
[6] D. MacDonald, D.L. Hunter, K. Kelly, and N. Jan, J. Phys. A **25**, 1429 (1992).
[7] P.M. Lam, Phys. Rev. B **42**, 4447 (1990).
[8] B. Li, N. Madras and A.D. Sokal (unpublished).
[9] A.J. Barrett and D.L. Tremain, Macromolecules **20**, 1687 (1987), and references therein.
[10] A.J. Barrett and A. Pound, J. Phys. A **13**, 1811 (1980).
[11] B. Duplantier, Phys. Rev. Lett. **57**, 941 (1986); B. Duplantier and H. Saleur, *ibid.* **57**, 3179 (1986).
[12] J.L. Cardy, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. Lebowitz (Academic, New York, 1987), Vol. 11, p.55.
[13] S.A. Colby, D.S. Gaunt, G.M. Torrie, and S.G. Whittington, J. Phys. A **20**, L515 (1987).
[14] C.E. Soteros, J. Phys. A., **25**, 3153 (1992).
[15] D. Zhao, T. Lookman, and K. De'Bell, Phys. Rev. A **42**, 4591 (1990).
[16] A.J. Guttmann, J. Phys. A **20**, 1839 (1987).
[17] K. De'Bell, T. Lookman, and S.G. Whittington, Phys. Rev. A **41**, 682 (1990).
[18] G.A. Baker, Jr. and D.L. Hunter, Phys. Rev. B **7**, 3377 (1973).